Exercise Sheet 4 due 13 November 2014

1. Airy functions

Consider a triangular well with infinite potential for $z \le 0$ and $V(z) = e\mathcal{E} z$ for z > 0. Find the lowest three eigenstates when the electric field is $\mathcal{E}=0.2$ V/Å. What are the lowest three eigenstates when the field is doubled?

2. infinite potential well in electric field

Consider an infinite potential well of width L=12 Å. Determine (numerically) the eigenfunctions and energies for the three lowest states for (i) zero electric field and (ii) in the presence of an electric field of 500 V/ μ m. Measure energies from the potential at the center of the infinite well. For each of the states, determine the probability of finding the electron in the left (-L/2 < z < 0) and the right (0 < z < L/2) half of the well.

3. Numerov method

Numerically calculate the solution of the Schrödinger equation with linear potential $e\mathcal{E} \times \text{with } \mathcal{E}=1 \text{ V/Å}$, for some energy E.

- i. Decide what units to use in your calculation
- ii. Integrate the Schrödinger equation to the left, starting 15 Å to the right of the classical turning point. What are reasonable values φ_0 and φ_1 for starting the integration, when you have no routine to calculate the Airy functions? How do the solutions depend on this choice? How do they depend on the energy E?
- iii. Use the Airy functions to start the numerical integration, integrate from 15 Å to the right of the classical turning point and continue for 30 Å. Compare your numerical result to the exact solution as a function of grid spacing *h*. Plot the error versus *h* for the simple integration and the Numerov method.
- iv. Numerically integrate the Schrödinger equation as above. Then starting from the last two points you have calculated, integrate backwards (towards larger x) into the classically forbidden region. Compare the two solutions.